LETTER TO THE EDITOR

A basis of cranking operators for the pairing-plus-quadrupole model

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Abstract. We investigate the RPA normal-mode coordinates in the pairing-plus-quadrupole model, with an eye on simplifying the application of large amplitude collective motion techniques. At the Hartree-Bogoliubov minimum, the RPA modes are exactly the cranking operators of the collective coordinate approach. We examine the possibility of representing the self-consistent cranking operator by linear combinations of a limited number of one-body operators. We study the Sm nuclei as an example, and find that such representations exist in terms of operators that are state-dependent in a characteristic manner.

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The selection of proper collective variables is an important problem in the study of large amplitude collective motion. In the usual Constrained Hartree-Fock (CHF) or Hartree-Fock-Bogoliubov (CHFB) calculations, the collective subspaces are generated by a small number of one-body constraint (also called cranking) operators which are most commonly taken to be of the multipole form ($r^L Y_{LK}$). In realistic calculations of processes such as fission, the number of coordinates to describe the full nuclear dynamics can easily become larger than can be dealt with in satisfactory manner, and a method to determine the optimal combination needs to be devised. Even assuming that such a method exists, there is no *a priori* reason to limit oneself to multipole operators, and the cranking operators should be determined by the nuclear collective dynamics itself, from the set of all one-body operators. This is clearly a difficult task, and one would like to be able to select a small group of operators, and find the optimal combination of these operators at each point of the collective surface.

In our past work, we have investigated a theory of adiabatic large amplitude collective motion as a method to generate self-consistent collective subspaces (see reference [1] and references therein). The key ingredient of the method is the self-consistent determination of the constraint operator, and as such it may provide an answer to the selection question discussed above. Using the local harmonic version (LHA) of the theory [1], we have recently embarked on a study of the properties of large amplitude collective motion in systems with pairing. We have dealt with two simple models: a semi-microscopic model of nucleons interacting through a pairing force, coupled to a single harmonic variable [2] and a fully microscopic $O(4)$ model which may

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be regarded as a simplified version of the pairing-plus-quadrupole (P+Q) Hamiltonian [3]. It has turned out that the self-consistent collective coordinate obtained by the LHA accounts quite well for the exact dynamics of these models. We have also shown that the CHFB calculations using the mass-quadrupole operator as the constraint operator can result in incorrect results [3]. It is not immediately obvious that we can extrapolate the conclusions reached in these models to fully realistic nuclear problems. Within the time-dependent Hartree-Bogoliubov (TDHB) approximation, the dynamics of these models is described by a modest number of degrees of freedom ($4 \sim 12$). For realistic problems in heavy nuclei, on the other hand, we need to deal with millions of degrees of freedom! In this letter, we report the first attempts to study such realistic nuclear problems.

In the LHA, the collective path (or collective surface for more than one coordinate) is determined by solving the CHFB problem with a cranking operator which is self-consistently determined by the local RPA. Since this procedure requires us to solve the RPA at each point on the collective path, it will be very useful if the RPA eigenvectors can be approximated by taking linear combinations of a small number of one-body operators. This means that we can restrict the RPA diagonalisation to this small space, rather than deal with the full millions-by-millions RPA matrix. Such a scenario has been examined in reference [4] and in reference [5] for the HF problem in ^{28}Si, and a strong radial and spin dependence of self-consistent cranking operators was found. However, since the model space had only six degrees of freedom and the pairing degrees of freedom were neglected, the results can not be directly generalised to heavy nuclei. Here we perform a similar analysis for the P+Q model. Since the model is known to be able to realistically describe collective phenomena involving both pairing and quadrupole degrees of freedom [6, 7], we expect that the same choice for the set of one-body operators should work for other realistic Hamiltonians as well.

Baranger and Kumar analysed in great detail the collective motion in the P+Q model assuming that the collective variables are the mass quadrupole operators [7]. Thus, they reduced the large number of two-quasiparticle (2qp) degrees of freedom (of the order of a thousand) into only two "collective" coordinates, β and γ. However, our previous study of the $O(4)$ model [3] suggests that even for such simple Hamiltonians the self-consistent collective coordinate is not as trivial as it seems to be. In this letter we report the first result for the P+Q model and show that the normal-mode coordinate of the random-phase approximation (RPA) is quite different from the mass quadrupole operator. This is especially true when the system is deformed.

For the P+Q model, the Hartree-Bogoliubov (HB) ground state can be specified by 6 parameters (Δ_n, Δ_p, λ_n, λ_p, β and γ). The TDHB equations can be shown to be equivalent to Hamilton's equations of motion [8]. The underlying classical Hamiltonian can be written, up to second order in coordinates and momenta, as

$$\mathcal{H} \equiv \langle \Psi | H - \mu N | \Psi \rangle \approx E_0 + \frac{1}{2} B^{\alpha\beta} \pi_\alpha \pi_\beta + \frac{1}{2} C_{\alpha\beta} \xi^\alpha \xi^\beta \ , \tag{1}$$

in terms of the canonical variables (ξ, π) [8]. Here each of the indices $(\alpha, \beta, \cdots)$ indicates a pair of 2qp indices $(ij, kl, \cdots)$. We adopt the standard tensor notation where a repeated upper and lower index indicates a summation. The mass and curvature parameters are

$$B^{\alpha\beta} = E_\alpha \delta_{\alpha\beta} - 2 \sum_\rho \chi_\rho S^{(\rho)}_\alpha S^{(\rho)}_\beta \ , \qquad C_{\alpha\beta} = E_\alpha \delta_{\alpha\beta} - 2 \sum_\rho \chi_\rho R^{(\rho)}_\alpha R^{(\rho)}_\beta \ . \tag{2}$$

Here $R^{(\rho)}$ and $S^{(\rho)}$ represent the hermitian and anti-hermitean components, respectively, of the pairing and quadrupole operators,

$$R^{(\rho)} = \sum_{\alpha} R^{(\rho)}_{\alpha} \left((a^{\dagger} a^{\dagger})_{\alpha} + \text{h.c.} \right) \ , \qquad S^{(\rho)} = \sum_{\alpha} S^{(\rho)}_{\alpha} \left((a^{\dagger} a^{\dagger})_{\alpha} - \text{h.c.} \right) \ , \tag{3}$$

where the scattering terms $(a^{\dagger} a)$ are omitted. Following reference [7], we multiply the quadrupole operators by a factor α_{τ}^2 with $\alpha_n = (2N/A)^{1/3}$ and $\alpha_p = (2Z/A)^{1/3}$, and also reduce the quadrupole matrix elements between the states of the upper shell by a factor $\zeta = (\mathcal{N}_{\rm L} + \frac{3}{2})/(\mathcal{N} + \frac{3}{2})$, where $\mathcal{N}$ is the oscillator quantum number operator and $\mathcal{N}_{\rm L}$ is the number of quanta in the lower shell. Thus, the modified quadrupole operators are defined as $Q_{2K} \equiv (Q_{2K})_n + (Q_{2K})_p$, with $(Q_{2K})_n = \alpha_n^2 \zeta (r^2 Y_{2K})_n$ and $(Q_{2K})_p = \alpha_p^2 \zeta (r^2 Y_{2K})_p$ (which we shall refer to as "the quadrupole operators"). The RPA equation is solved by diagonalisation of the Hamiltonian (1). This can be implemented by a (linear) transformation to normal coordinates (q^{μ}),

$$q^{\mu} = f^{\mu}_{,\alpha} \xi^{\alpha}, \qquad \xi^{\alpha} = g^{\alpha}_{,\mu} q^{\mu} \ , \tag{4}$$

where $f^{\mu}_{,\alpha}$ and $g^{\alpha}_{,\mu}$ are just coefficients of linear transformation. These can be also identified as $\partial q^{\mu}/\partial \xi^{\alpha}$ and $\partial \xi^{\alpha}/\partial q^{\mu}$ for the general point transformation, $q^{\mu} = f^{\mu}(\xi)$ and $\xi^{\alpha} = g^{\alpha}(q)$, when we study large excursions from equilibrium [1]. In the case of a single collective coordinate, the path is determined by solving the CHB equation with the cranking operator $q^1 = f^1(\xi)$. A similar set of equations has been also obtained by other adiabatic time-dependent mean-field theories [9].

The solution of the RPA equation

$$C_{\alpha\gamma} B^{\gamma\beta} f^{\mu}_{,\beta} = (\Omega^{\mu})^2 f^{\mu}_{,\alpha} \ , \tag{5}$$

involves the diagonalisation of the RPA matrix $C_{\alpha\gamma} B^{\gamma\beta}$ whose dimension is equal to the number of active 2qp degrees of freedom. For separable forces, this can be simplified by solving a dispersion relation. In general, however, the RPA diagonalisation requires extensive computational resources. Now let us approximate an eigenvector using a certain set of one-body operators $\{O^{(i)}\}$:

$$\bar{f}_{,\alpha} = \sum_{i} C_i O^{(i)}_{\alpha} \ , \tag{6}$$

where $O^{(i)}_{\alpha}$ indicate the 2qp matrix elements of operator $O^{(i)}$ as in equation (3). Then, instead of the full RPA equation (5), we obtain a projected RPA equation

$$\bar{M}^{ij} C^n_j = \left(\bar{\Omega}^n \right)^2 \bar{N}^{ij} C^n_j \ , \tag{7}$$

which determines the coefficients C^n_i, with

$$\bar{M}^{ij} \equiv O^{(i)}_{\alpha} B^{\alpha\beta} C_{\beta\gamma} B^{\gamma\delta} O^{(j)}_{\delta} \ , \qquad \bar{N}^{ij} \equiv O^{(i)}_{\alpha} B^{\alpha\beta} O^{(j)}_{\beta} \ . \tag{8}$$

The dimension of the matrices $\bar{M}^{ij}$ and $\bar{N}^{ij}$ is equal to the number of one-body operators $\{O^{(i)}\}$. Therefore, if we can approximate the RPA eigenvectors by using a small number of operators, it will significantly reduce the computational task.

A criterion for good projection may be given by the closeness of the projected RPA frequencies $\bar{\Omega}$ to the real RPA frequencies Ω. Another criterion is the smallness of the quantity δ,

$$\delta = f_{,\alpha} B^{\alpha\beta} \left(f_{,\beta} - \bar{f}_{,\beta} \right) \ . \tag{9}$$

If we normalise f^{μ} as $f^{\mu}_{,\alpha} B^{\alpha\beta} f^{\nu}_{,\beta} = \delta^{\mu\nu}$, we find $0 \leq \delta \leq 1$ with $\delta = 0$ corresponding to the exact projection and $\delta = 1$ to the case where $\bar{f}$ is orthogonal to f.

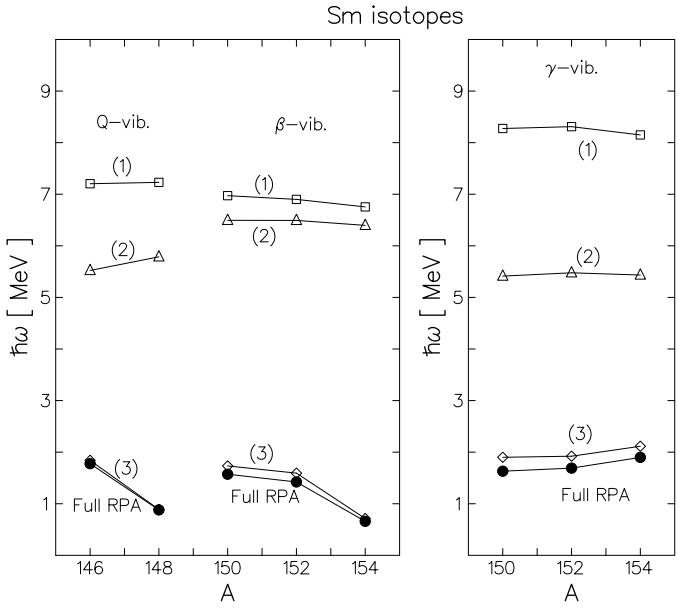

Figure 1. Calculated excitation energies of quadrupole, β and γ vibrations for even-even Sm isotopes. Note that the ground states of ^{146,148}Sm are spherical. The closed circles indicate the RPA results while the open symbols are the results of projected RPA calculations. See the main text for the difference between (1), (2) and (3).

We have performed calculations for several heavy isotopes. Here we report the numerical results for even-even Sm isotopes (A=146∼154). The form of the P+Q model is that discussed in the second and third of the series of papers by Baranger and Kumar [7]. The model space and the parameters, such as the spherical single-particle energies, the pairing and quadrupole force strengths, are taken from table 1 in the third paper. The equilibrium parameters (β, γ, Δ, λ) are found to agree with table 2 of the same paper. The ground states of ^{146,148}Sm are spherical ($\beta = 0$) and the others have prolate shapes ($\beta > 0, \gamma = 0$).

Figure 1 shows the excitation energies (RPA frequencies) of β and γ vibrations, obtained by the RPA and projected RPA calculations. For the projected RPA calculations, we have adopted three different sets of one-body operators. The first and simplest choice is to use the operators appearing in the separable forces, the pairing and quadrupole operators, P_τ, $P^\dagger_\tau$, $(Q_{2K})_\tau$ ($\tau = n, p$). This choice is denoted as (1) in the figure. In this case the projected RPA matrices of equation (8) are two dimensional for spherical nuclei and for γ vibrations, while they are six dimensional for the β vibrations. The calculated frequencies are $7 \sim 8$ MeV which are $5 \sim 6$ MeV larger than the corresponding RPA frequencies. In the second set, labelled as (2), we increase the number of operators. We keep both the pairing and quadrupole operators, but include two additional quadrupole operators with "monopole" radial dependence, $(r^0 Y_{2K})_\tau$. We also include the hexadecapole operators, $(r^4 Y_{4K})_\tau$, and the rank-2 spin-dependent operators, $([r^0 Y_2 \times \mathbf{s}]^{(2)}_K)_\tau$, $([r^2 Y_2 \times \mathbf{s}]^{(2)}_K)_\tau$. As far as the frequencies are concerned, we can see some improvement over the case (1) for spherical and the γ vibrations in deformed nuclei, though they are still much higher than the

Table 1. Calculated values of δ, equation (9), for the projected RPA solutions for Sm isotopes. The columns (1), (2), (3), (1-a) and (1-b) represent the different projections (see text). For the spherical nuclei (^{146,148}Sm), there is no distinction between β and γ vibrations.

A	β vibration					γ vibration				
	(1)	(1-a)	(1-b)	(2)	(3)	(1)	(1-a)	(1-b)	(2)	(3)
146	0.271	0.132	0.225	0.421	0.009					
148	0.243	0.131	0.184	0.314	0.0003					
150	0.602	0.499	0.519	0.632	0.026	0.610	0.342	0.507	0.685	0.092
152	0.497	0.346	0.433	0.526	0.020	0.616	0.279	0.472	0.691	0.081
154	0.513	0.117	0.437	0.534	0.002	0.636	0.208	0.426	0.679	0.052

real RPA frequencies. For the β vibrations, the inclusion of the additional rank-2 (and higher rank) operators seems not so important. Actually we see that the β vibrations are found to have a significant amount of monopole components. For the last set, denoted as (3), we adopt the same operators as (1) but each 2qp matrix element is weighted with a factor $(E_{2\mathrm{qp}})^{-2}$. This means that we employ a set of *state-dependent* one-body operators $\{\widetilde{O}^{(i)}\}$ defined by

$$\widetilde{O} \equiv \sum_{\alpha} \frac{O_\alpha}{(E_\alpha)^2} (a^\dagger a^\dagger)_\alpha + \mathrm{h.c.}\ . \tag{10}$$

The result of this projection is now almost identical to that of the full RPA.

In table 1, the quality of projection δ, equation (9), is listed. In the cases (1) and (2), where the RPA vectors are projected on the elementary operators, $\delta \gtrsim 0.25$ for ^{146,148}Sm and $\delta \gtrsim 0.5$ for the others. Therefore, roughly speaking, the one-body operators possess at most 75% (50%) of overlap with the real eigenvectors in spherical (deformed) nuclei. On the other hand, the projection (3) exhausts more than 90% of real eigenvectors even for the worst case. At first sight it may look strange that δ is larger for (2) than for (1), while the energy for (2) is lower. This is due to the fact that case (2) is dominated by certain neutron components. Since the relevant neutron 2qp energies are lower than those of protons, this proton-neutron asymmetry leads to a decrease in the frequency $\bar{\Omega}$ and at the same time an increase in δ. This is also a reflection of the poor quality of the approximation.

The figure and table indicate that it is very difficult to obtain sensible results by using elementary one-body operators (i.e., of the form (1) or (2)). This is mainly due to the fact that the RPA eigenvectors, when being projected onto elementary one-body operators, have unrealistically large amplitudes for high-lying 2qp components. In order to demonstrate this, we introduce a cut-off energy Λ_{cut} for the 2qp matrix elements, i.e., $O^{(i)}_\alpha = 0$ for $E_\alpha > \Lambda_{\mathrm{cut}}$. We then perform the projected RPA calculation with the truncated one-body operators from set (1). The resulting values δ are listed in table 1 for $\Lambda_{\mathrm{cut}} = 5$ MeV (1-a) and for 10 MeV (1-b). We see that the major contributions to the RPA modes come from the 2qp components with $E_{2\mathrm{qp}} < 5$ MeV. We thus conclude that the superiority of the projection (3) simply comes from its being capable of suppressing the unnecessary high-energy components by the factor $(E_{2\mathrm{qp}})^{-2}$. This suppression factor is not arbitrary, but can be derived from the following simple argument. If we have a single-mode separable force $H = -(1/2)\chi RR$

(assuming no coupling among different modes), we can analytically determine the RPA eigenvectors, $f^{\mu}_{,\alpha} \propto R_\alpha/((E_\alpha)^2 - (\Omega^\mu)^2)$. In the limit that $\Omega^\mu \ll E_{2\mathrm{qp}}$, the projection on $f_{,\alpha} \propto R_\alpha/(E_\alpha)^2$ gives the exact answer.

Let us examine the projection (3) in more detail. For spherical Sm nuclei, the RPA eigenvector is of isoscalar character and can be approximated as $\bar{f} \approx (\widetilde{Q}_2)_n + (\widetilde{Q}_2)_p$ where the tilde indicates that the matrix elements include the suppression factor as in equation (10). For deformed nuclei, where the collectivity of the vibrational states is smaller than for spherical nuclei and the pairing modes can mix with the quadrupole ones, the situation is more complex. Taking ^{154}Sm as an example, the eigenvectors of β and γ vibrations are

$$\bar{f}^{\beta-\mathrm{vib}} = (\widetilde{Q}_{20})_n + 0.91(\widetilde{Q}_{20})_p - 0.48\widetilde{P}_n - 0.44\widetilde{P}_p + 0.085\widetilde{P}^\dagger_n - 0.14\widetilde{P}^\dagger_p \ , \tag{11}$$

$$\bar{f}^{\gamma-\mathrm{vib}} = (\widetilde{Q}_{22})_n + 0.87(\widetilde{Q}_{22})_p \ . \tag{12}$$

For the β vibration, we find a significant mixing with the monopole pairing modes.

In conclusion, we have examined the possibility of expressing the self-consistent cranking operator in terms of a limited set of one-body operators. It seems very difficult to approximate the normal-mode vectors with use of elementary one-body operators. This difficulty disappears, however, when we use a small number of *state-dependent* one-body operators. This may reflect the importance of the self-consistent determination of the collective coordinates for large amplitude collective motion, because the coordinates now have a strong state-dependence as well. The structure of the self-consistent cranking operators is clearly changing when we move from spherical to deformed nuclei. For the study of large amplitude collective motion in heavy nuclei for which the diagonalisation of the RPA matrix becomes too time-consuming, the results of this paper may give a hint for a correct choice of a state-dependent basis of operators. The choice of a limited set of (state dependent) basis operators provides a practical way to solve the LHA through the projection. With the self-consistent cranking operators, the LHA should provide a significant improvement over the conventional CHFB calculation based on fixed cranking operators. Clearly we have not discussed the structure of the self-consistent cranking operator away from the minimum point. This will be the subject of a future publication.

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References

[1] Klein A, Walet N R and Do Dang G 1991 *Ann. Phys., NY* **208** 90
[2] Nakatsukasa T and Walet N R 1998 *Phys. Rev.* **C57** 1192
[3] Nakatsukasa T and Walet N R 1998 *Phys. Rev.* **C58** 3397
[4] Pelet J and Letourneux J 1977, *Nucl. Phys.* **A281** 277
[5] Do Dang G, Walet N R and Klein A 1994 *Phys. Lett.* **B322** 11
[6] Kisslinger L S and Sorensen R A 1960 *Mat. Fys. Medd. Dan. Vid. Selsk.* **32** No. 9
[7] Baranger M and Kumar K 1965 *Nucl. Phys.* **62** 113; 1968 *Nucl. Phys.* **A110** 490, **A110** 529, **A122** 241, **A122** (1968) 273
[8] Blaizot J P and Ripka G 1986 *Quantum Theory of Finite Systems*, (Cambridge, Massachusetts: The MIT Press)
[9] Ring P and Schuck P 1980 *Nuclear Many-Body Problems*, (New York: Springer Verlag)